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Final Report

Workshop on Nanocomposites

Award No. F49620-01-1-0480

Virginia Polytechnic Institute and State University

Submitted by M.W. Hyer

April 2004

This report summarizes the workshop held on the campus of Virginia Polytechnic Institute and State University September 12-13, 2001. The report consists of notes taken during the workshop by an appointed scribe that briefly describe the workshop format, and then summarize, in bullet form, the discussions that occurred. A list of attendees concludes this report.

Air Force Workshop on NanoMechanics

September 12-13, 2001

Virginia Polytechnic Institute and State University (VPI&SU), Blacksburg, VA

Workshop Summary

Scope

The workshop was held VPI&SU, September 12-13, 2001, following the 16th Annual Technical Conference of American Society for Composites, September 12-13, Virginia Tech. The Air Force Office of Scientific Research (AFOSR) sponsored the workshop. The purpose of the workshop was to bring together experts to open a dialog among the researchers and program managers to describe and define/quantify the limits and benefits of modeling and testing of nano-reinforced composites. More specifically, the purpose was to outline DOD/NASA challenges and needs, together with brainstorming/initial strategizing of Air Force plan (short and long term).

The workshop was arranged to have briefing by the agency representatives on Wednesday (September 12) afternoon, followed by Invited Speakers' presentations and discussions on Thursday (September 13) morning, with the objective to define needed research directions in the area of nanomechanics and associated processing/morphology with specifics such as

- Current issues
- Specific directions
- Expected benefits
- Near and far term research efforts.

In order to facilitate a coherent discussion through out the workshop and to define Air Force's nanomechanics research needs/goals, the speakers were requested in advance to tailor their presentations to address the following topics/categories

1. Value and benefits of nanocomposites (observed and expected potential)
2. Modeling at the nano level (benefits, limits, and new technologies/techniques requirements)
3. Testing at the nano level (benefits, limits, and new technologies/techniques requirements)
4. Materials to explore in near term, long term
5. Strategy for the mechanics/composites community.

Speakers' presentations

The purpose of the speakers' presentations was to summarize the existing state of the art and define needed research directions that will allow the technology to be of benefit the Air Force. The speakers presented their work in two groups. The agency representatives summarized their briefings in the first group to address as they see the overall technology needs/challenges (Wednesday afternoon, Sept 12), followed by the invited speakers to

share their expertise in nano technology (Thursday morning, September 13). Following is the list of speakers invited to the workshop

Agency Perspectives

Tom Hahn, AFOSR	Air Force 6.1 perspective
Derek Lincoln, AFRL/MLBP	Air Force 6.2 perspective
Tom Gates, NASA-Langley	NASA perspective
Jim Thomas, NRL	Navy perspective
Michael Sennett*	Army perspective (could not attend)

General Presentations

Barry Farmer, AFRL/MLBP	Molecular modeling
Tom Hahn, UCLA	Blending nanoparticles in polymers
Alexander Moravsky, MER Corp.	Carbon nanotube processing
Satish Kumar*, Georgia Tech	Blending nanotube in polymer and polymer fibers
Rod Ruoff*, Northwestern Univ	Characterization of nanoreinforcements
Yuris Dzenis*, Univ of Nebraska	Spinning nanofibers
G. P. Tandon, UDRI	Continuum mechanics modeling
Don Paul, Univ of Texas, Austin	Polymer nanocomposites
Mary Boyce*, MIT	Nanocomposites modeling
Tia Benson Tolle, AFRL/MLBC	Nanosilicate reinforced polymers

* Could not attend due to the travel problems caused by the September 11, 2001 incident

The electronic version of the above presentations is requested from the speakers. Following the speakers' presentations, the comments of the speakers and attendees are gathered through a round-the-room discussion. The summary of the discussion is categorized below under five topics (same as given in advance to the speakers), which will be useful in defining Air Force's research directions/objectives/goals in nanomechanics.

The summary of the discussion comments in each topic are presented below as follows

1. Value and Benefits of nanocomposites

- Look into functional properties (maintain mechanical, maintain processing characteristics)
- Multiple applications, diverse
- Improved performance (various) properties, surface smoothness
- Great potential exists
- Reinforcements are important
- Potential is anticipated, yet often not anticipated (e.g., flammability)
- Still unexplored behavior (extreme environment, etc.)
- More than just nanocomposites; nanotech/nanomaterials, too

2. Modeling – Nano Level

- Need modeling
- Tools exist (continuum)
 - with built-in assumptions
 - interface characteristics unknown
- Don't always know what the material is--constituent size, interface
- Need molecular modeling to know what's going on in molecular level
- Connectivity of existing models in different scales needed
- Modeling at some level desired by experimentalists
- Models can show potential benefits, assurance of direction
- Fracture mechanics methods exist, not yet tapped into
- Find out what are we modeling? Properties, etc.

3. Testing at Nano Level

- Need to assess distributions interface
- Need characterization of the nano constituents
- Need characterization of the nanocomposite
- Scales of testing/measurement techniques is as important as scaling of models
- Model behavior at nano and bulk
- Combinational chem. analysis
- Required for processing optimization
- Testing is difficult to obtain (e.g., of NIH), perhaps need dedicated test house...No one has all the necessary test capabilities
- Test methods for nanocomp/modified resins are not standardized, as opposed to PMC (D2O vs. D3O)
- Role of national labs?

4. Materials to Explore

- Constituents: platelets better than spheres, fibers for mechanical props
- CNT need to be tailored for the polymer
- Synthesis, functionalization, availability of CNT an issue
- Dispersion, adhesion, processing are key issues

- Need to define nanoscale (vs. nanofiber)
- Nano constituent effect on matrix must be understood
- Bulk vs. confined material (E, ...)
- Plethora of materials...and increasing number of variety of nanoreinforcement is a problem
- Range of nanoconstituents available to assess potential
- Geometries $\rightarrow \infty$: [ages (poss)]
- Nanoporous materials
- Material selection as a function of desired outcome
- Materials with atomically-controlled interfaces
- Not necessarily looking at NC (nanocomposite) as replacements for PMC, but as added constituents... \therefore behavior of nanomod poly \neq behavior of nano and PMC

5. Strategy for Nanomechanics

- Do theoretical props of nano constituents translate to composite properties?
- Not everyone needs to do everything
 - Need to go to molecular mechanics
- Need to reduce our scale of observation
- Want better sense of direction, focus
 - Start with conventional composite theory
- Maybe too early for a strategy
- Promote commonality in research projects
- Forum like this of value to the community
- Test standards
- Advocate diverse groups getting together
- Encourage/stress multidisciplinary approach
- Multiscale approach
- Multifunctional materials approach
- Niche = nano with respect to structural method, OMCs
- Plan future Nano Sessions within ACS - "Tom Hahn's Website" will be useful to provide a forum for future interaction

Conclusions

It appears to be apparent from the above discussion comments that there is a need for a selection of a very few materials systems (nano reinforcement and matrix material) to pursue a thorough and systematic investigation to understand dispersion mechanism, interface adhesion with appropriate characterization tools, standard test methods, and multiscale modeling covering the nano-scale (to understand interface behavior) to the material continuum

List of Attendees

NanoComposites Workshop, VPI&SU, September 12-13, 2001

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